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Maximum Cellular Boolean Functions and Perfect Gray Codes [1]

A. J. Goldman and B. K. Bender

(January 28, 1963)

I. A Boolean function of n variables, considered as a subset of the discrete unit n-cube B_n, is called *cellular* if each of its connected components is a face of B_n. Hamming's determination of optimal binary single-error-detecting codes is generalized to a characterization of all proper cellular functions with the greatest possible number of elements. II. An analysis is made of a class of Gray codes (Hamiltonian circuits on B_n) with certain special properties, e.g., admitting for $0 \leq d \leq n$ a partition into 2^{n-d} subpaths each forming a d-dimensional face of B_n.

1. Introduction

Let B_n be the set of vertices of the unit cube in n-dimensional space; equivalently, B_n is the set of all binary sequences [2] of length n. A *Boolean function* of n variables is simply a subset [3] of B_n.

Call two vertices of B_n *neighbors* if they differ in precisely one position. A Boolean function f is called *connected* if, given any two vertices X, X' in f, there exists a sequence

$$X = X_1, X_2, X_3, \ldots, X_{k-1}, X_k = X'$$

of members of f such that X_i and X_{i+1} are neighbors for $1 \leq i \leq k-1$. It is easy to show that if f is not connected, then it has a unique partition into maximal connected subsets called its *components*; [4] if f *is* connected, the unique component consists of f itself.

The relevance of these concepts to the simplification of Boolean functions is as follows. By a *cell* of a Boolean function f, we mean a face [5] of B_n which lies wholly in f. A *cover* of f is a collection C of cells of f such that each vertex of f lies in at least one cell from C. Each cell of f is assigned a *cost* in a manner which need not be described here, and the cost of a cover C is defined to be the sum of the costs of the cells of C. The problem of finding a minimum-cost cover of f is then identical with the "Problem of Quine" [6] of finding a simplest "normal disjunctive form" for f, a problem of practical interest (for example) in the design of switching circuits. From the fact that each cell is connected and therefore lies in a single component of f, it follows that any cover of f is a disjoint union of covers of the components of f and conversely; in particular any minimum-cost cover of f is a disjoint union of minimum-cost covers of the components of f, and conversely. That is, the Boolean simplification problem for a function f which is not connected, can be split into independent "smaller" subproblems by splitting f into its components. Such a decomposition is clearly likely to be helpful in attacking the simplification problem.[7]

In this context it is natural to ask how many components a Boolean function of n variables can possibly have. This question will be answered in section 2, in which we also investigate the structure of the *maximum* disconnected functions of n variables, i.e., those with the greatest possible number of components.

The discussion above also makes it natural to focus attention on classes of Boolean functions f such that the simplification problem for each *component* of f is especially easy. One such class is that of *isolated* functions, those with only single vertices of B_n as components. An isolated Boolean function can be identified with a single-error-detecting binary code, and our characterization in section 2 of *maximum* isolated functions (those with as many vertices as possible), which verifies a conjecture of Chittenden,[8] is essentially the same as an "optimal code" characterization due to Hamming.[9]

For all methods of "cost" assignment suggested for the Problem of Quine, the faces F of B_n have the property that $\{F\}$ is the unique minimum-cost cover of F. Thus the class of Boolean functions f, such that each component of f is a cell of f, is one of the

[1] Supported in part by the National Science Foundation, Grant No. G-7579.

[2] A sequence is *binary* if each of its terms is either 0 or 1.

[3] The equivalence of this definition with alternative ones is well-known in the field and will not be discussed here.

[4] Define a binary relation on f: XRX' holds if X and X' are in a connected subset of f. Then R is an equivalence relation and the components of f are the corresponding equivalence classes.

[5] A d-dimensional *face* of the "discrete cube" B_n is obtained by fixing the (binary) values of $n-d$ of the n coordinates.

[6] W. V. Quine, The Problem of Simplifying Truth Functions, Amer. Math. Monthly **59** (1952), pp. 521–531. There is no reason here to cite the extensive literature on this topic.

[7] Of course the labor required to determine the components should be taken into account.

[8] E. W. Chittenden, On the minimal representation of Boolean functions, Transactions of the Third Conference of Arsenal Mathematicians, U.S. Army Office of Ordnance Research Rept. No. 58-2, p. 134.

[9] R. W. Hamming, Error detecting and error correcting codes, Bell System Tech. J. **29** (1950), pp. 147–160. Our proof by induction is quite different from Hamming's, and this approach may be of independent interest.

classes mentioned in the last paragraph. Such functions will be called *cellular*, and in section 3 we determine the structure of maximum cellular functions (those other than B_n, with as many vertices as possible). This generalization of Hamming's theorem from isolated functions to cellular functions, is the main new result of the paper.

A *Gray code* on B_n, in the language of graph theory, is a Hamiltonian circuit of the graph formed from B_n by the "neighbor" relation.[9a] In section 4, the inductive approach introduced earlier (in sec. 2) is employed to establish the existence of Gray codes with certain special properties, e.g., admitting a partition into 2^{n-d} subpaths each forming a d-dimensional face of B_n. These "perfect" Gray codes turn out to coincide with what were called the "conventional" Gray codes by Gilbert,[9b] who described them in different notation using essentially the same recursive construction. The treatment in section 4, besides giving additional detail on the structure of these Hamiltonian circuits, highlights their geometric aspects in a way which may be better suited to some readers' mathematical intuition than is the strictly arithmetic treatment associated in this context with the phrase "reflected binary."[9c] It may be of interest that this material was developed from purely geometric considerations, in ignorance of "reflected binary."

2. Maximum Disconnected and Isolated Functions

We begin with a simple lemma:

LEMMA 1. *There is at least one maximum disconnected function of* n *variables which is isolated.*

For the proof, observe first that because the number of Boolean functions of n variables is finite, a maximum disconnected function f must exist. Now form a function f' by deleting all but one member from every component of f. Clearly f' is isolated, and it must be maximum disconnected since it has the same number of components as does f.

In what follows, it will be convenient to associate to each Boolean function f of $k+1$ variables, two Boolean functions f_0 and f_1 of k variables each, called the *projections*[9d] of f. f_0 is obtained by dropping the final 0 from each member of f which ends in 0, while f_1 is obtained by dropping the final 1 from each member of f which ends in 1. Note that

$$|f| = |f_0| + |f_1|, \tag{1}$$

where $|f|$ denotes the number of members of f.

LEMMA 2. *If* M_n *is the maximum number of components of a Boolean function of* n *variables, then* $M_n \leq 2^{n-1}$.

This is clear for $n=1$; assume it true for $n=k$ and consider the case $n=k+1$. Lemma 1 guarantees the existence of a maximum disconnected function f of $k+1$ variables which is isolated; then eq (1) shows that $M_{k+1} = |f_0| + |f_1|$. It is easy to see that f_0 and f_1 are also isolated, so that for $i=0$ and $i=1$, $|f_i|$ is the number of components of f_i. Therefore $|f_i| \leq M_k$, and so we have $M_{k+1} \leq 2M_k$. But $M_k \leq 2^{k-1}$ by the induction hypothesis, so that $M_{k+1} \leq 2^k$ and the induction proof is complete.

We now define two special Boolean functions of n variables; $f(n)$ consists of those members of B_n with an *even* number (possibly zero) of 1's among their entries,[9e] while $g(n)$ consists of those members of B_n with an *odd* number of 1's among their entries.

THEOREM 1. *The functions* f(n) *and* g(n), *which form a partition of* B_n, *are the only maximum isolated Boolean functions of* n *variables.* $M_n = 2^{n-1}$.

Part of the proof is trivial; it is clear that $f(n)$ and $g(n)$ *are* isolated, and that they form a partition of B_n. Since $f(n)$ and $g(n)$ each have 2^{n-1} members and thus the same number of components, we have $M_n \geq 2^{n-1}$ and the equality follows by lemma 2.

It only remains to show that if h is *any* maximum isolated function of n variables, then h is either $f(n)$ or $g(n)$. This is clear for $n=1$; suppose it true for $n=k$ and consider the case $n=k+1$. As in the proof of lemma 2,

$$2^k = M_{k+1} = |h| = |h_0| + |h_1| \leq M_k + M_k = 2^k,$$

where we have used the fact that h_0 and h_1 are isolated because h is. Since equality holds throughout the last display, h_0 and h_1 each have exactly M_k components. The induction hypothesis leads to four possibilities:

$$h_0 = f(k) \text{ and } h_1 = f(k),$$
$$h_0 = g(k) \text{ and } h_1 = g(k),$$
$$h_0 = f(k) \text{ and } h_1 = g(k),$$
$$h_0 = g(k) \text{ and } h_1 = f(k).$$

The first two possibilities are incompatible with the fact that h is isolated, the third yields $h = f(k+1)$, and the fourth yields $h = g(k+1)$; these conclusions follow from the identity [10]

$$h = (h_0 \times \{0\}) \cup (h_1 \times \{1\}) \tag{2}$$

valid for Boolean functions of $k+1$ variables. Thus the induction proof is complete.

[Jack Edmonds (NBS Operations Research Section) has observed that B_n can be regarded as a bipartite graph, and has given the following (unpublished) generalization of theorem 1: For a connected bipartite graph which has a connected regular subgraph containing all its vertices, the sets of the

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[9a] Some authors use "Gray code" to mean any path or circuit in the linear graph formed by B_n.

[9b] E. C. Gilbert, Gray codes and paths on the N-cube, Bell System Tech. J. **37** (1958).

[9c] See for example I. Flores, Reflected number systems, Trans. Inst. Radio Eng. Vol. **EC-5** (1956).

[9d] In the switching-circuit literature f_0 and f_1 would be called the *residues* of f with respect to the "last" of the $k+1$ Boolean variables.

[9e] That is, a vertex $X = (x_1, x_2, \ldots, x_n)$ of B_n is in $f(n)$ if and only if $\sum_{i=1}^{n} x_i$ is even.

[10] $h_0 \times [0]$ is obtained by adjoining a 0 at the end of each member of h_0. The multiplication sign refers to the Cartesian-product representation of B_{k+1} as $B_k \times [0, 1]$.

unique bipartition are the only maximum isolated sets of vertices.]

One might conjecture that a maximum disconnected Boolean function is necessarily isolated. A counter-example for $n=1$ is provided by B_1 itself. The next theorem shows that this is the only counter-example.

THEOREM 2. *For* $n>1$, *every maximum disconnected function of* n *variables is isolated.*

To prove this, let f be a maximum disconnected function of $n>1$ variables. As in the proof of lemma 1, form f' by deleting all but one member from each component of f. Since f' is isolated and has the same number of components as f, it follows from theorem 1 that f' is either $f(n)$ or $g(n)$. Without loss of generality assume $f'=f(n)$. If $f\neq f'$, then f includes at least one vertex Y of $g(n)$.

One neighbor X_1 of Y is obtained by changing just the first entry of Y, while a second neighbor X_2 is obtained by changing just the second entry of Y. Since X_1 and X_2 are in $f(n)=f'$ and thus in f, and both are neighbors of the same vertex Y of f, it follows that the elements X_1 and X_2 of f' lie in the same component of f. This however contradicts the construction of f'; we conclude that $f=f'$, so that f is isolated.

3. Maximum Cellular Functions

Recall that a Boolean function f is called *cellular* if each component of f is a cell of f; different components may be cells of different dimensions. Cellular functions are a natural generalization of isolated functions.

THEOREM 3. *Let* $\mathrm{F_d}$ *be a* d-*dimensional face of* $\mathrm{B_n}$, $0\leq \mathrm{d}<\mathrm{n}$. *There exists a Boolean function* $\mathrm{f(n;F_d)}$ *of* n *variables with* $\mathrm{F_d}$ *as a component,* $2^{\mathrm{n-d-1}}$ *components in all, and every component a* d-*dimensional cell. The complement* $\mathrm{g(n;F_d)}$ *of* $\mathrm{f(n;F_d)}$ *in* $\mathrm{B_n}$ *also has* $2^{\mathrm{n-d-1}}$ *components, each a* d-*dimensional cell.*

These functions $f(n;F_d)$ and $g(n;F_d)$ can be regarded as the analogs, for cellular functions, of the functions $f(n)$ and $g(n)$ (defined before theorem 1) for isolated functions. For example our later results will imply as a special case that these functions (for various F_d) give the only solutions to the problem of constructing a cellular function with as many components as possible under the restriction that every component is a d-dimensional cell; theorem 1 is the particular instance $d=0$.

We prove the theorem by explicitly constructing $f(n;F_d)$ and verifying its properties. For simplicity assume F_d consists of all members $(x_1, x_2, \ldots, x_n)$ of B_n such that $x_i=0$ for $d+1\leq i\leq n$; any other d-dimensional face can be treated similarly. The cube B_n can be written as a Cartesian product $B_d\times B_{n-d}$, i.e., a binary sequence of length n is uniquely expressible as a sequence of length d followed by one of length $n-d$. With this notation, we use the functions introduced before theorem 1 to define

$$f(n;F_d)=\mathsf{U}\{B_d\times\{Z\}: Z\epsilon f(n-d)\}=B_d\times f(n-d).$$

Each set $B_d\times\{Z\}$ is easily shown to be a d-dimensional face of B_n and is therefore connected; F_d itself is obtained as $B_d\times\{0_{n-d}\}$ where 0_{n-d} is a sequence of $n-d$ zeros. Since $f(n-d)$ has 2^{n-d-1} members (see theorem 1), there are 2^{n-d-1} sets $B_d\times\{Z\}$. To see that these sets are the *components* of $f(n;F_d)$, it suffices to observe that any two members Z, Z' of the isolated function $f(n-d)$ differ in at least two positions, so that no member of $B_d\times\{Z\}$ can be a neighbor of any member of $B_d\times\{Z'\}$.

The complement of $f(n-d)$ in B_{n-d} is the isolated set $g(n-d)$ which has 2^{n-d-1} members. Therefore the complement of $f(n;F_d)$ in B_n is

$$g(n;F_d)=\mathsf{U}\{B_d\times\{Z\}: Z\epsilon g(n-d)\}=B_d\times g(n-d)$$

whose components are the 2^{n-d-1} d-dimensional faces $B_d\times\{Z\}$ of B_n with $Z\epsilon g(n-d)$. Thus theorem 3 is proved.

Before proving the next theorem, it is convenient to collect several elementary facts as a lemma.

LEMMA 3. *Let* $\mathrm{f_0}$ *and* $\mathrm{f_1}$ *be the projections of a cellular function* f *of* k+1 *variables. Then*

(a) *if* h *is a component of* f, *then either* $\mathrm{h_0}=\phi$ *or* $\mathrm{h_1}=\phi$ *or* $\mathrm{h_0}=\mathrm{h_1}$,

(b) *for* i=0 *and* i=1, *the components of* $\mathrm{f_1}$ *are the nonvoid projections* $\mathrm{h_1}$ *of the components* h *of* f,

(c) $\mathrm{f_0}$ *and* $\mathrm{f_1}$ *are cellular if nonempty, and*

(d) *if component* p *of* $\mathrm{f_0}$ *meets component* q *of* $\mathrm{f_1}$, *then* $\mathrm{p=q=h_0=h_1}$ *for some component* h *of* f.

To begin the proof, let h be any component of f. Since f is cellular, for some d there exist $S_h\subset\{1,2,\ldots, k,k+1\}$ with $k+1-d$ members, and a binary sequence $\{c_i: i\epsilon S_h\}$, such that h consists of all members $(x_1, \ldots, x_{k+1})$ of B_{k+1} obeying

$$x_i=c_i \text{ for all } i\epsilon S_h.$$

If $k+1\epsilon S_h$ and $c_{k+1}=0$, then $h_1=\phi$ and h_0 consists of all members $(x_1, \ldots, x_k)$ of B_k such that

$$x_i=c_i \text{ for all } i\epsilon S_h-\{k+1\}.$$

If $k+1\epsilon S_h$ and $c_{k+1}=1$, then $h_0=\phi$ and h_1 consists of all members $(x_1, \ldots, x_k)$ of B_k such that

$$x_i=c_i \text{ for all } i\epsilon S_h-\{k+1\}.$$

If $k+1\epsilon\{1, \ldots, k+1\}-S_h$, then h is the disjoint union of the set of members of B_{k+1} such that

$$x_{k+1}=0,\ x_i=c_i \text{ for all } i\epsilon S_h$$

and the set of members of B_{k+1} such that

$$x_{k+1}=1,\ x_i=c_i \text{ for all } i\epsilon S_h;$$

thus $h_0=h_1$ consists of all members of B_k such that

$$x_i=c_i \text{ for all } i\epsilon S_h.$$

This proves (a) of the lemma, and also shows that h_0 and h_1 are faces of B_k and therefore cells of f_0 and f_1 respectively.

To prove (b) of the lemma for $i=0$ (the proof for $i=1$ is similar), it now suffices to show that if h_0 and h_0^* are nonempty projections of *distinct* components h and h^* of f, then no member X of h_0 is a neighbor of any member X^* of h_0^*. If such a "neighboring" occurred, however, then the member $X\times\{0\}$ of h would be a neighbor of the member $X^*\times\{0\}$ of h^*, which is impossible. Thus (b) holds; (c) follows from (b) and the fact (proved incidentally in the last paragraph) that the projections of a face are again faces.

Now suppose a component p of f_0 and a component q of f_1 have a member X in common. By (b), there exist components h_p and h_q of f such that $(h_p)_0=p$ and $(h_q)_1=q$. Thus $X\times\{0\}$ is in h_p and its neighbor $X\times\{1\}$ is in h_q, so that $h_p=h_q=h$, say. It follows from (a) that $p=q$, so (d) is proved.

THEOREM 4. *The maximum number of members in a cellular Boolean function of* n *variables (other than* B_n*) is* 2^{n-1}. *For* $0\leq d<n$ *and each* d*-dimensional face* F_d *of* B_n, $f(n; F_d)$ *is the only cellular function with* 2^{n-1} *members which has* F_d *as a component.*

This is clear for $n=1$; assume it true for $n=k$ and consider the case $n=k+1$. Let V_{k+1} be the maximum number of members in a cellular function, other than B_{k+1}, of $k+1$ variables; V_k is defined similarly. It follows from theorem 3 that $V_{k+1}\geq 2^k$. To prove the opposite inequality, let f be a cellular function of $k+1$ variables with V_{k+1} members. If either of f_0 or f_1 is B_k then by (d) of lemma 3 the other must be empty, since otherwise we would have $f_0=f_1=B_k$ and thus $f=B_{k+1}$. Thus if $f_0=B_k$ then $f_1=\phi$ and $f=B_k\times\{0\}$, while if $f_1=B_k$ then $f_0=\phi$ and $f=B_k\times\{1\}$; in either case $V_{k+1}=|f|=2^k$. If both f_0 and f_1 are *proper* subsets of B_k then by the inductive hypothesis and (c) of lemma 3 we have

$$V_{k+1}=|f|=|f_0|+|f_1|\leq V_k+V_k=2^{k-1}+2^{k-1}=2^k, \quad (3)$$

completing the proof that $V_n=2^{n-1}$ for all n.

Now let F_d be a d-dimensional face of B_{k+1}, where $0\leq d<k+1$, and let f be a cellular Boolean function of $k+1$ variables with 2^k members and F_d as a component. For simplicity we again use the representation $B_{k+1}=B_d\times B_{k+1-d}$ and assume $F_d=B_d\times\{0_{k+1-d}\}$, where 0_{k+1-d} is a sequence of $k+1-d$ zeros.[10a]

If $f_0=B_k$ then (see the last paragraph)

$$f=B_k\times\{0\}=f(k+1; F_k)=f(k+1; F_d)$$

where the last equation holds since F_d is to be a component and $B_k\times\{0\}$ has F_k as sole component. If $f_1=B_k$ then (see the last paragraph) $f_0=\phi$, which is impossible since f_0 contains the nonempty set [11] $(F_d)_0=B_d\times\{0_{k-d}\}$. So we can assume f_0 and f_1 are *proper* cellular functions of k variables; by (3), f_0 and f_1 each have 2^{k-1} members, so that by inductive hypothesis and (b) and (c) of lemma 3,

$$f_0=f(k; (F_d)_0).$$

In the next paragraph we will show that $f_1=B_k-f_0$; it follows that

$$f_1=g(k; (F_d)_0)$$

and thus by eq (2) that

$$f=(f(k; (F_d)_0)\times\{0\})\cup(g(k; (F_d)_0)\times\{1\}).$$

From the explicit formulas for $f(n; F_d)$ and $g(n; F_d)$ given in the proof of theorem 3, we have

$$\begin{aligned} f(k; (F_d)_0)\times\{0\}&=[\cup\{B_d\times\{Z\}: Z\epsilon f(k-d)\}]\times\{0\}\\ &=\cup\{B_d\times\{Z\times\{0\}\}: Z\epsilon f(k-d)\}\\ &=B_d\times(f(k-d)\times\{0\}), \end{aligned}$$

where we have used the fact $(F_d)_0=B_d\times\{0_{k-d}\}$, and similarly

$$g(k; (F_d)_0)\times\{1\}=B_d\times(g(k-d)\times\{1\}).$$

Thus

$$\begin{aligned} f&=B_d\times[(f(k-d)\times\{0\})\cup(g(k-d)\times\{1\})]\\ &=B_d\times f(k+1-d)=f(k+1; F_d), \end{aligned}$$

as was to be proved.

It remains to prove that $f_1=B_k-f_0$. Since f_0 and f_1 each have 2^{k-1} members, it suffices to prove $f_1\subset B_k-f_0$, i.e., that no component p of f_0 meets any component q of f_1. If such a meeting occurred, then by (d) of lemma 3 we have $p=q=h_0=h_1$ for some component h of f, and by (b) of lemma 3 p is a component of f_1 as well as f_0. By (c) of lemma 3, f_0 and f_1 are both cellular, and by induction hypothesis there is only one cellular function of k variables with 2^{k-1} members having p as a component. Therefore $f_1=f_0$, so that $(F_d)_0$ is a component of f_1 as well as of $f_0=f(k; (F_d)_0)$. Thus

$$\begin{aligned} &B_d\times\{0_{k-d}\}\times B_1\\ &\quad=[B_d\times\{0_{k-d}\}\times\{0\}]\cup[B_d\times\{0_{k-d}\}\times\{1\}]\\ &\quad=[(F_d)_0\times\{0\}]\cup[(F_d)_0\times\{1\}]\\ &\quad\subset[f_0\times\{0\}]\cup[f_1\times\{1\}]=f; \end{aligned}$$

since the first set is a face of B_{k+1} which properly contains $F_d=B_d\times\{0_{k+1-d}\}$, we have a contradiction to the hypothesis that F_d is a component of f. This completes the proof of theorem 4.

The last two theorems yield the following statement:

COROLLARY. *A cellular Boolean function of* n *variables (other than* B_n*) with the maximum number of members has all its component cells of the same dimension,* d, *and its complement is again such a function (with the same* "d"). *There are* $2\binom{n}{d}$ *such functions*

[10a] For consistency it is important that this representation and assumption match the corresponding ones in the proof of theorem 3, so that the explicit formula for $f(n; F_d)$ introduced in that proof can validly be used below.

[11] For $k=d$, the Cartesian product reduces to B_k.

for each $d<n$, *and thus in all there are* $2(2^n-1)$ *cellular functions of* n *variables with the maximum number of members.*

The number $2\binom{n}{d}$ is obtained by dividing the number $2^{n-d}\binom{n}{d}$ of d-dimensional faces of B_n by the number 2^{n-d-1} of these faces appearing in a maximum cellular function.

4. Perfect Gray Codes

An even simpler proof of lemma 2 and theorem 1, in section 2, can be given if we take as known the existence of a Gray code, i.e., an enumeration $\{X_i : 1\leq i\leq 2^n\}$ of the members of B_n such that X_i and X_{i+1} are neighbors for $1\leq i\leq 2^n=N$, and X_N and X_1 are neighbors. From this it is obvious that an isolated set cannot contain both X_i and X_{i+1}, or both X_N and X_1, and so has at most 2^{n-1} members. It is also clear that the sets

$$F(n)=\{X_i : i \text{ is even}\},\quad G(n)=\{X_i : i \text{ is odd}\},$$

if they are isolated, are the unique maximum isolated functions of n variables. But the defining property of a Gray code shows that the parity of the number of 1's in X_i is opposite to that for X_{i+1}, so that the number of 1's in every member of $F(n)$ has the same parity, while the opposite parity holds for all members of $G(n)$. Thus either $F(n)=f(n)$ and $G(n)=g(n)$, or $F(n)=g(n)$ and $G(n)=g(n)$; since $f(n)$ and $g(n)$ are easily proved to be isolated the same is true of $F(n)$ and $G(n)$, so that the conclusions of lemma 2 and theorem 1 have been established.

The inductive technique used in section 2 to prove lemma 2 and theorem 1, and in section 3 to prove theorem 4, can also be employed to establish the existence of a Gray code on B_n for all $n\geq 1$. We shall actually prove a stronger result, namely the existence of a class of Gray codes (to be called *perfect*) with certain additional properties which have been found helpful in aiding visualization. For example ((a) of theorem 5), for each d with $1\leq d\leq n$ such a code partitions into 2^{n-d} successive subpaths, each essentially a perfect Gray code on some d-dimensional face of B_n. Also a rather explicit description can be given of the positions (in a perfect Gray code) of the n neighbors of any member of B_n whose position in the code is given; see corollary 1 to theorem 7.

For $0\leq d\leq n$ and $1\leq j\leq 2^{n-d}=N(n-d)$, it is convenient to define

$$S_j^d=\{i : (j-1)2^d<i\leq j2^d\},$$

a subset of $\{1, 2, 3, \ldots, 2^n=N(n)\}$. For any subset S of $S_{2\nu-1}^d$, we call the subset

$$S'=\{i : (2\nu-1)2^{d+1}+1-i\epsilon S\}$$

of $S_{2\nu}^d$ the *reflection* of S in $(2\nu-1)2^d$, while for any subset S of $S_{2\nu}^d$ the *reflection* S' of S in $(2\nu-1)2^d$ is the subset of $S_{2\nu-1}^d$ defined by the same formula. Here $0\leq d<n$ and $1\leq\nu\leq N(n-d-1)$. Familiarity with the reflected binary number system should provide partial motivation for this definition.

For any enumeration $\{X_i : 1\leq i\leq 2^n=N(n)\}$ of the members of B_n, and any subset T of $\{1, 2, 3, \ldots, N(n)\}$, let

$$X(T)=\{X_i : i\epsilon T\}.$$

The enumeration will be called a *perfect Gray code* if, for each d with $0\leq d<n$, for each ν with $1\leq\nu\leq N(n-d-1)$, and for each subset S of either $S_{2\nu-1}^d$ or $S_{2\nu}^d$ such that $X(S)$ is a δ-dimensional face of B_n for some $\delta\leq d$, the set $X(S')$ corresponding to the reflection S' of S in $(2\nu-1)2^d$ is also a δ-dimensional face, and furthermore $X(S)\cup X(S')$ is a $(\delta+1)$-dimensional face.

To indicate the implications of this fairly complicated definition, we collect some properties of perfect Gray codes in the next theorem, in which the notation

$$F_j^d=X(S_j^d)$$

is employed.

THEOREM 5. *If* $\{X_i : 1\leq i\leq N(n)\}$ *is a perfect Gray code on* B_n, *then*

(a) F_j^d *is a* d*-dimensional face,*

(b) $F_j^d\cup F_{j+1}^d$ *is a* $(d+1)$*-dimensional face,*

(c) $F_j^d\cup F_{N(n-d)+1-j}^d$ *is a* $(d+1)$*-dimensional face.*

First (a) will be proved for $0\leq d\leq n$. It is clearly true for $d=0$; assume it true for $d=k<n$, and consider the case $d=k+1$. Observe that

$$S_j^{k+1}=S_{2j-1}^k\cup S_{2j}^k$$

and that each disjunct is the other's reflection in $(2j-1)2^d$. Since by induction hypothesis F_{2j-1}^k is a k-dimensional face, it follows from the definition of "perfectness" that F_j^{k+1} is a $(k+1)$-dimensional face. This completes the inductive proof of (a).

To prove (c), it now suffices to observe that $S_{N(n-d)+1-j}^d$ is the reflection of S_j^d in $N(n-1)$. To prove (b), factor j as

$$j=2^a b<N(n-d)\quad (a\geq 0,\ b \text{ odd})$$

and observe that S_j^d is a subset of S_b^{a+d} whose reflection in $b2^{a+d}$ is S_{j+1}^d.

By setting $d=0$ in (b) of theorem 5, and also in (c) with $j=1$, we see that a perfect Gray code is indeed a Gray code. An imperfect Gray code on B_3, where for example F_1^2 is not a face, is given by

$$\begin{array}{llll}(0,0,0), & (1,0,0), & (1,0,1), & (1,1,1)\\ (1,1,0), & (0,1,0), & (0,1,1), & (0,0,1).\end{array}$$

Next we prove the existence of a perfect Gray code on B_n; in analogy with theorem 3 it will in fact be shown that such a code can be chosen to "begin" with any preassigned face F of B_n. Because the formal proof which follows is somewhat forbidding, we summarize the geometric idea first: B_n is considered as made up of two copies of B_{n-1} (for simplicity, $B_{n-1}\times\{0\}$ and $B_{n-1}\times\{1\}$), the first copy containing F; the perfect Gray code on B_n is constructed by choosing an appropriate perfect Gray code on B_{n-1} (which exists by induction hypothesis), tracing it out in $B_{n-1}\times\{0\}$ and then tracing it out *in*

reverse order in $B_{n-1}\times\{1\}$. When $F=\phi$ this construction agrees with one given by Gilbert (op. cit. in footnote 9b), and if iterated for $n>1$ it gives the particular perfect Gray codes which Gilbert termed the "conventional" ones.[12]

THEOREM 6. *Let* F *be a* d(0)*-dimensional face of* B_n, *with* $0\leq d(0)\leq n$. *There exists a perfect Gray code on* B_n *for which* $F_1^{d(0)}=F$.

This is clearly true for $n=1$; assume it true for $n=k$ and consider the case $n=k+1$. If $d(0)=k+1$, so that $F=B_{k+1}$, then we are simply to prove the existence of a perfect Gray code on B_{k+1}, which will follow from the analysis for $d(0)\leq k$. So suppose $d(0)\leq k$; to simplify notation we can assume $F\subset B_k\times\{0\}$, so that F is given in terms of its projection F_0 as $F=F_0\times\{0\}$.

It is easy to prove that F_0 is a $d(0)$-dimensional face of B_k. By inductive hypothesis, there is a perfect Gray code $\{Y_i: 1\leq i\leq N(k)\}$ on B_k for which

$$F_0=\{Y_i: 1\leq i\leq 2^{d(0)}\}.$$

Now define an enumeration $\{X_i: 1\leq i\leq N(k+1)\}$ of B_{k+1} by

$$X_i=Y_i\times\{0\} \text{ if } 1\leq i\leq N(k),$$
$$X_i=Y_{N(k+1)+1-i}\times\{1\} \text{ if } N(k)<i\leq N(k+1).$$

We shall show that this enumeration is the desired perfect Gray code. The following notation will be used:

$$X(S)=\{X_i: i\epsilon S\},$$
$$Y(R)=\{Y_i: i\epsilon R\},$$
$$S_j^d=\{i: (j-1)2^d<i\leq j2^d\} \quad (0\leq d\leq k+1,\ 1\leq j\leq N(k+1-d)),$$
$$R_j^d=\{i: (j-1)2^d<i\leq j2^d\} \quad (0\leq d\leq k,\ 1\leq j\leq N(k-d)),$$
$$F_j^d=X(S_j^d),$$
$$G_j^d=Y(R_j^d).$$

First, it is clear that

$$F=F_0\times\{0\}=G_1^{d(0)}\times\{0\}=F_1^{d(0)},$$

as desired. Second, consider any d with $0\leq d\leq k$, any ν with $1\leq\nu\leq N(k-d)$, and any subset S of either $S_{2\nu-1}^d$ or $S_{2\nu}^d$ such that $X(S)$ is a δ-dimensional face of B_{k+1} for some $\delta\leq d$. Let S' be the reflection of S in $(2\nu-1)2^d$. The proof will be completed by showing that $X(S')$ is a δ-dimensional face, and $X(S)\cup X(S')$ a $(\delta+1)$-dimensional face. It will be assumed that S is a subset of $S_{2\nu-1}^d$ rather than $S_{2\nu}^d$; the details for the other case are analogous.

Suppose first that $\nu\leq N(k-d-1)$. Then $X_i=Y_i\times\{0\}$ for each $i\ \epsilon S\cup S'$. Therefore

$$X(S)=Y(S)\times\{0\},\quad X(S')=Y(S')\times\{0\},$$
$$X(S)\cup X(S')=(Y(S)\cup Y(S'))\times\{0\}.$$

The first of these equations shows that $Y(S)$ is a δ-dimensional face of B_k, so that $Y(S')$ is a δ-dimensional face and $Y(S)\cup Y(S')$ a $(\delta+1)$-dimensional face; the second and third equations then yield the same results for $X(S)$ and $X(S)\cup X(S')$.

Next suppose $\nu>N(k-d-1)$ and $d<k$. Then

$$X_i=Y_{N(k+1)+1-i}\times\{1\}$$

for each $i\epsilon S\cup S'$. Let R and R' be the respective reflections of S and S' in $N(k)$, so that

$$X(S)=Y(R)\times\{1\},\quad X(S')=Y(R')\times\{1\}$$
$$X(S)\cup X(S')=(Y(R)\cup Y(R'))\times\{1\}.$$

The first of these equations shows that $Y(R)$ is a δ-dimensional face of B_k. It is readily verified that R' is the reflection of R in

$$[2(2^{k-d}-(\nu-1))-1]2^d,$$

so that $Y(R')$ is a δ-dimensional face and $Y(R)\cup Y(R')$ a $(\delta+1)$-dimensional face; the second and third equations then yield the same results for $X(S')$ and $X(S)\cup X(S')$.

The final situation is $d=k$, so that $\nu=1$. Here

$$X_i=Y_i\times\{0\} \text{ for } i\epsilon S,$$
$$X_i=Y_{N(k+1)+1-i}\times\{1\} \quad \text{for } i\epsilon S'$$

so that

$$X(S)=Y(S)\times\{0\}\quad X(S')=Y(S)\times\{1\},$$
$$X(S)\cup X(S')=Y(S)\times\{0,\ 1\},$$

and the result follows.

The next theorem gives more detail on the structure of perfect Gray codes.

THEOREM 7. *Let* $\{X_i: 1\leq i\leq N(n)\}$ *be a perfect Gray code on* B_n, *and* T *a set of* $2^{\delta+1}$ *elements of* $\{1, 2, \ldots, N(n)\}$. *If* X(T) *is a* $(\delta+1)$*-dimensional face of* B_n, *then there exists* d *with* $\delta\leq d<n$, ν *with* $1\leq\nu\leq N(n-d-1)$, *and a partition* $T=S\cup S'$ *such that* S *is a subset of either* $S_{2\nu-1}^d$ *or* $S_{2\nu}^d$, S′ *is the reflection of* S *in* $(2\nu-1)2^d$, *and* X(S) *is a* δ*-dimensional face.*

This is clear for $n=1$; assume it true for $n=k$, and consider the case $n=k+1$. By (a) of Theorem 5, F_1^k is a k-dimensional face of B_{k+1}, and to simplify notation we may assume $F_1^k=B_k\times\{0\}$. Thus $F_2^k=B_k\times\{1\}$. If we define Y_i to be the projection $(X_i)_0$ for $1\leq i\leq N(k)$, then by (c) of theorem 5 $X_{N(k+1)+1-i}\epsilon B_k\times\{1\}$ is a neighbor of $X_i\epsilon B_k\times\{0\}$, which implies that $Y_i=(X_{N(k+1)+1-i})_1$. That is,

$$X_i=Y_i\times\{0\} \text{ for } 1\leq i\leq N(k)$$
$$X_i=Y_{N(k+1)+1-i}\times\{1\} \text{ for } N(k)<i\leq N(k+1).$$

That $\{Y_i: 1\leq i\leq N(k)\}$ is a perfect Gray code on B_k follows easily from the corresponding fact for $\{X_i: 1\leq i\leq N(k+1)\}$ and the first of the last two equations.

Suppose first that $T\subset S_1^k$. Then

$$X(T)=Y(T)\times\{0\}$$

[12] In theorem 6 below we write $d(0)$ instead of d_0 for typographical convenience.

and so $Y(T)$ is a $(\delta+1)$-dimensional face of B_k. By induction hypothesis there exist d with $\delta \le d < k$, ν with $1 \le \nu \le N(k-d-1)$, and a partition $T = S \cup S'$ such that S is a subset of either $S^d_{2\nu-1}$ or $S^d_{2\nu}$, S' is the reflection of S in $(2\nu-1)2^d$, and $Y(S)$ is a δ-dimensional face of B_k. Thus

$$X(S) = Y(S) \times \{0\}$$

is a δ-dimensional face of B_{k+1}, as desired.

Next suppose $T \subset S^k_2$. Let T' be the reflection of T in $N(k)$; then

$$X(T) = Y(T') \times \{1\}$$

and so $Y(T')$ is a $(\delta+1)$-dimensional face of B_k. By induction hypothesis there exist d with $\delta \le d < k$, ν with $1 \le \nu \le N(k-d-1)$, and a partition $T' = S \cup S'$ such that S is a subset of either $S^d_{2\nu-1}$ or $S^d_{2\nu}$, S' is the reflection of S in $(2\nu-1)2^d$, and $Y(S)$ is a δ-dimensional face of B_k. Let R and R' be the respective reflections of S and S' in $N(k)$, so that we have a partition $T = R \cup R'$, and

$$X(R) = Y(S) \times \{1\}$$

is a δ-dimensional face of B_{k+1}. Since R is a subset of either $S^d_{2\mu-1}$ or $S^d_{2\mu}$ where

$$\mu = 2^{k-d} - \nu + 1,$$

and R' is the reflection of R in $(2\mu-1)2^d$, again matters are as desired.

Finally, suppose T meets both S^k_1 and S^k_2. Then $X(T)$, as a $(\delta+1)$-dimensional face of B_{k+1} which meets both $B_k \times \{0\}$ and $B_k \times \{1\}$, can easily be shown to have the form

$$X(T) = F \times \{0,1\}$$

where F is a δ-dimensional face of B_k. Say $F = Y(S)$ where $S \subset S^k_1$. It follows that

$$T \cap S^k_1 = S, \quad T \cap S^k_2 = S'$$

where S' is the reflection of S in $N(k)$. Since $X(S) = F \times \{0\}$ is a δ-dimensional face of B_{k+1}, the proof is complete.

COROLLARY 1. *Let* $\{X_i : 1 \le i \le N(n)\}$ *be a perfect Gray code on* B_n. *Then the* n *neighbors of* X_1 *are the* $\{X_{k(d)} : 0 \le d < n\}$ *defined by*

$$k(d) = (2\nu(d)-1)2^{d+1} + 1 - i$$

where $\nu(d)$ *is defined by*

$$(2\nu(d)-2)2^d < i \le 2\nu(d)2^d.$$

This follows from theorem 7 with $\delta = 0$.

COROLLARY 2. *Let* $\{X_i : 1 \le i \le N(n)\}$ *be a perfect Gray code on* B_n. *If* $j(1)$ *and* $j(2)$ *are distinct but have the same parity, then no member of* $F^\delta_{j(1)}$ *is a neighbor of a member of* $F^\delta_{j(2)}$.

For, suppose a member X_i of $F^\delta_{j(1)}$ and a member X_k of $F^\delta_{j(2)}$ were neighbors, so that

$$(j(1)-1)2^\delta + 1 \le i \le j(1)2^\delta,$$

$$(j(2)-1)2^\delta + 1 \le k \le j(2)2^\delta,$$

and by corollary 1 there exist d with $0 \le d < n$, and $\nu = \nu(d)$, such that

$$i + k = (2\nu-1)2^{d+1} + 1$$

and

$$(\nu-1)2^{d+1} + 1 \le i \le \nu 2^{d+1},$$

which imply that

$$(\nu-1)2^{d+1} + 1 \le k \le \nu 2^{d+1}.$$

On the one hand, we have

$$\begin{aligned}(j(2)-1)2^\delta + 1 - j(1)2^\delta &\le k - i \\ &= (i+k) - 2i \\ &\le [(2\nu-1)2^{d+1} + 1] \\ &\quad - 2[(\nu-1)2^{d+1} + 1],\end{aligned}$$

so that

$$[j(2) - j(1) - 1]2^\delta + 1 \le 2^{d+1} - 1$$

and therefore

$$j(2) - j(1) < 2^{d+1-\delta} + 1.$$

On the other hand by interchanging i with k and $j(1)$ with $j(2)$ in this argument, we obtain

$$j(1) - j(2) < 2^{d+1-\delta} + 1.$$

Since the hypotheses on $j(1)$ and $j(2)$ imply $|j(2) - j(1)| \ge 2$, the last two displays imply that $d + 1 - \delta > 0$. But then we would have

$$\begin{aligned}[(j(1)-1)2^\delta + 1] + [(j(2)-1)2^\delta + 1] &\le i + k \\ &= (2\nu-1)2^{d+1} + 1 \\ &= i + k \\ &\le j(1)2^\delta + j(2)2^\delta,\end{aligned}$$

so that

$$[j(1) + j(2) - 2]2^\delta + 2 \le (2\nu-1)2^{d+1} + 1 \le [j(1) + j(2)]2^\delta,$$

$$[j(1) + j(2) - 2]2^\delta < (2\nu-1)2^{d+1} < [j(1) + j(2)]2^\delta,$$

$$j(1) + j(2) - 2 < (2\nu-1)2^{d+1-\delta} < j(1) + j(2),$$

with the hypotheses implying that the middle term (which lies between the consecutive even integers constituting the extreme terms) is an even integer. Since this is impossible, the corollary is proved.

Just as the existence of ordinary Gray codes provides an alternative approach to the material of section 2 (see the beginning of the present section), so the existence and properties of perfect Gray codes

provide an alternative approach to the material of section 3. Suppose for example that F_d is a d-dimensional face of B_n, with $0 \leq d < n$. Then by theorem 6 there is a perfect Gray code on B_n with $F_d = F_1^d$, and theorem 3 can be quickly proved by setting

$$f(n; F_d) = \cup\{F_j^d : 1 \leq j \leq N(n-d),\ j \text{ is odd}\},$$
$$g(n; F_d) = \cup\{F_j^d : 1 \leq j \leq N(n-d),\ j \text{ is even}\}$$

and invoking the last corollary (with d as δ) together with (a) of theorem 5.

We conclude by showing that "essentially" there is only one perfect Gray code on B_n, which must therefore be the "conventional" one mentioned earlier. To make this precise, observe that as a "discrete cube," B_n has as its natural group of symmetries the hyperoctahedral group $\mathcal{C}_n$ whose $(n!)2^n$ elements can be represented as the ordered pairs (σ, π) where σ is a subset of $\{1, 2, 3, \ldots, n\}$ and π is a permutation of $\{1, 2, 3, \ldots, n\}$. The operation of (σ, π) on a member $X = (x_1, \ldots, x_n)$ of B_n is the member X' defined by

$$x'_j = 1 - x_{\pi(j)} \text{ if } j \in \sigma,$$
$$x'_j = x_{\pi(j)} \text{ if } j \in \{1, 2, 3, \ldots, n\} - \sigma.$$

If $\{X_i : 1 \leq i \leq N(n)\}$ and $\{X'_i : 1 \leq i \leq N(n)\}$ are perfect Gray codes on B_n, we call them *equivalent* in case (with an obvious notation)

$$(\sigma, \pi)(X_i) = X'_i \text{ for } 1 \leq i \leq N(n)$$

for some (σ, π) in $\mathcal{C}_n$.

THEOREM 8. *Any two perfect Gray codes on* B_n *are equivalent.*

This is clear for $n = 1$; assume it true for $n = k$, and consider the case $n = k+1$. Let $\{X_i : 1 \leq i \leq N(k+1)\}$ and $\{X'_i : 1 \leq i \leq N(k+1)\}$ be perfect Gray codes on B_{k+1}. By theorem 5 $X(S_1^k)$ and $X'(S_1^k)$ are k-dimensional faces of B_{k+1}, so that there exist elements r and t of $\{1, 2, \ldots, k+1\}$, and numbers c and c' each either zero or one, for which

$$X(S_1^k) = \{X : X \in B_{k+1},\ x_r = c\},$$
$$X'(S_1^k) = \{X : X \in B_{k+1},\ x_t = c'\}.$$

Therefore one-to-one correspondences between B_k and each of $X(S_1^k)$ and $X'(S_1^k)$, are set up by the functions

$$g : X(S_1^k) \to B_k, \quad g' : X'(S_1^k) \to B_k$$

defined by

$$g(X) = (x_{\rho(1)}, x_{\rho(2)}, \ldots, x_{\rho(k)}),$$
$$g'(X) = (x_{\tau(1)}, x_{\tau(2)}, \ldots, x_{\tau(k)})$$

where $X = (x_1, \ldots, x_{k+1})$ and the permutations ρ and τ of $\{1, 2, \ldots, k+1\}$ are given by

$$\rho(j) = j \text{ if } j < r, \quad \rho(j) = j+1 \text{ if } r \leq j \leq k, \quad \rho(k+1) = r,$$
$$\tau(j) = j \text{ if } j < t, \quad \tau(j) = j+1 \text{ if } t \leq j \leq k, \quad \tau(k+1) = t.$$

It is trivial to verify that g transforms each d-dimensional face of B_{k+1} which lies wholly in $X(S_1^k)$ into a d-dimensional face of B_k, while g' does the same for those faces of B_{k+1} which lie wholly in $X'(S_1^k)$. Therefore

$$\{g(X_i) : 1 \leq i \leq N(k)\} \text{ and } \{g'(X'_i) : 1 \leq i \leq N(k)\}$$

are perfect Gray codes on B_k, so by induction hypothesis there exist a subset σ of $\{1, 2, \ldots, k\}$ and a permutation π of $\{1, 2, \ldots, k\}$ such that

$$(\sigma, \pi)(g(X_i)) = g'(X'_i) \text{ for } 1 \leq i \leq N(k).$$

If x_{ij} and x'_{ij} denote the jth entries of X_i and X'_i respectively, then this can be written as

$$x'_{i,\tau(j)} = 1 - x_{i,\rho\pi(j)} \text{ if } j \in \sigma$$
$$x'_{i,\tau(j)} = x_{i,\rho\pi(j)} \quad \text{if } j \in \{1, 2, \ldots, k\} - \sigma$$

for $1 \leq j \leq k$ and $1 \leq i \leq N(k)$.

Now form the permutation π' of $\{1, 2, \ldots, k+1\}$ defined by $\pi'(t) = r$ and

$$\pi'(j) = \rho\pi\tau^{-1}(j) \text{ for } j \neq t,$$

as well as the subset σ' of $\{1, 2, \ldots, k+1\}$ defined by

$$\sigma' = \tau(\sigma) \cup \{t\} \text{ if } c \neq c',$$
$$\sigma' = \tau(\sigma) \text{ if } c = c'.$$

Then it follows easily that

$$(\sigma', \pi')(X_i) = X'_i \text{ for } 1 \leq i \leq N(k),$$

and this remains true for $N(k) < i \leq N(k+1)$ because

$$x_{N(k+1)+1-i,\,j} = x_{ij} \text{ if } j \neq r,$$
$$x_{N(k+1)+1-i,\,r} = 1 - x_{ir},$$
$$x'_{N(k+1)+1-i,\,j} = x'_{ij} \text{ if } j \neq t,$$
$$x'_{N(k+1)+1-i,\,t} = 1 - x'_{it}$$

for $1 \leq i \leq N(k)$. Thus the two given perfect Gray codes on B_{k+1} are equivalent.

It is a pleasure to acknowledge helpful suggestions by K. Goldberg and E. Johnson (NBS Numerical Analysis Section) and R. Kirsch (NBS Components and Techniques Section).

(Paper 67B2–94)

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The Meaning of Betti's Reciprocal Theorem

C. Truesdell

(February 5, 1963)

It is demonstrated that Betti's reciprocal theorem represents a criterion for the existence of a stored-energy function.

It was remarked long ago [1][1] that Betti's reciprocal theorem, familiar in the linearized theory of elasticity, remains valid for infinitesimal strain superimposed upon an arbitrarily strained state of a hyperelastic material, and recently a proof was published [2]. The true significance of Betti's theorem, however, lies in its being a *criterion for the existence of a stored-energy function.*

Indeed, the differential equations and stress boundary conditions to be satisfied by the superimposed displacement field $\mathbf{u}$ are [3]

$$(A_{km}{}^{\alpha\beta}u^m{}_{;\beta})_{;\alpha}=\rho_{\mathrm{R}}(\ddot{u}_k-b^*{}_k),\quad A_{km}{}^{\alpha\beta}u^m{}_{;\beta}n_{\mathrm{R}\alpha}=t^*{}_{\mathrm{R}k}, \tag{1}$$

where ρ_{R} is the density in the reference configuration, $\mathbf{b}^*$ and $\mathbf{t}^*_{\mathrm{R}}$ are the excesses of external body force and surface traction, respectively, above those acting on the given strained state, $\mathbf{n}_{\mathrm{R}}$ is the outward unit normal in the reference configuration, and the semicolon denotes the total covariant derivative. The coefficients $A_{km}{}^{\alpha\beta}$ are defined directly from the stress-strain relation of the elastic material, not assumed to be hyperelastic:

$$T_{\mathrm{R}k}{}^{\alpha}=\mathfrak{h}_k{}^{\alpha}(x^m{}_{,\beta}),\ A_{km}{}^{\alpha\beta}(x^p{}_{,\gamma})=\frac{\partial\mathfrak{h}_k{}^{\alpha}}{\partial x^m{}_{,\beta}} \tag{2}$$

$\mathbf{T}_{\mathrm{R}}$ being the first Piola-Kirchhoff stress tensor [4]. In taking the stress-strain relation in the form $(2)_1$, we refrain from imposing the principle of material indifference, so that the results to be obtained remain valid also for theories somewhat more general than elasticity. Since an underlying deformation is laid down and fixed, the quantities $x^p{}_{,\gamma}$ are given functions of position. Thus the components $A_{km}{}^{\alpha\beta}$ are given, fixed functions of positions, and (1) is a linear differential equation for $\mathbf{u}$.

Let $\bar{\mathbf{b}}^*$ and $\bar{\mathbf{t}}^*_{\mathrm{R}}$ correspond to another infinitesimal deformation $\bar{\mathbf{u}}$ superimposed upon the same given, underlying strained state. Then

$$(A_{km}{}^{\alpha\beta}\bar{u}^m{}_{;\beta})_{;\alpha}=\rho_{\mathrm{R}}(\ddot{\bar{u}}_k-\bar{b}^*_k),$$

$$A_{km}{}^{\alpha\beta}\bar{u}^m{}_{;\beta}n_{\mathrm{R}\alpha}=\bar{t}^*_{\mathrm{R}k}. \tag{3}$$

Hence, by $(1)_1$,

$$\rho_{\mathrm{R}}(\ddot{u}_k-b^*_k)\bar{u}^k=(A_{km}{}^{\alpha\beta}u^m{}_{,\beta})_{;\alpha}\bar{u}^k,$$

$$=(A_{km}{}^{\alpha\beta}u^m{}_{,\beta}\bar{u}^k)_{;\alpha}-A_{km}{}^{\alpha\beta}u^m{}_{;\beta}\bar{u}^k{}_{;\alpha}. \tag{4}$$

Integration over a region $\mathscr{B}_{\mathrm{R}}$ in the reference configuration, followed by use of the divergence theorem and $(1)_2$, yields the following *Betti identity:*

$$\int_{\mathscr{B}_{\mathrm{R}}}\rho_{\mathrm{R}}(b^*_k-\ddot{u}_k)\bar{u}^k dV_{\mathrm{R}}+\oint_{\partial\mathscr{B}_{\mathrm{R}}}t^*_{\mathrm{R}k}u^k dS_{\mathrm{R}}$$

$$=\int_{\mathscr{B}_{\mathrm{R}}}A_{km}{}^{\alpha\beta}u^m{}_{,\beta}\bar{u}^k{}_{;\alpha}dV_{\mathrm{R}}. \tag{5}$$

Betti's reciprocal theorem consists in the assertion that in the sum on the left-hand side, barred and unbarred quantities may be interchanged. In order that this be possible, for all $\mathbf{u}$ and $\bar{\mathbf{u}}$ and for all regions $\mathscr{B}_{\mathrm{R}}$, it is necessary and sufficient that

$$A_{km}{}^{\alpha\beta}=A_{mk}{}^{\beta\alpha}, \tag{6}$$

for the ground state considered.

Thus far we have laid down a single ground state. If we now demand that Betti's theorem shall hold for infinitesimal deformation from an arbitrary underlying state of strain, we infer that (6) must hold as an identity in the argument $x^p{}_{,\gamma}$. This condition, by (2), is necessary and sufficient for the existence of a potential $\sum(x^m{}_{,\beta})$ such that

$$T_{\mathrm{R}k}{}^{\alpha}=\frac{\partial\sum(x^m{}_{,\beta})}{\partial x^k{}_{,\alpha}}. \tag{7}$$

Thus we have proved that *Betti's reciprocal theorem, for infinitesimal deformation from an arbitrary state of strain, provides a necessary and sufficient condition that an elastic material be hyperelastic.*

This result is only an interpretation of the familiar fact that a reciprocity theorem for solutions of a linear differential system is a necessary and sufficient condition for the system to be self-adjoint.

[1] Figures in brackets indicate the literature references at the end of this paper.

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(Paper 67B2–95)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
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Effect of Molecular Weight on Viscoelastic Properties of Polymers as Predicted by a Molecular Theory

Hansjörg Oser and Robert S. Marvin

(February 27, 1963)

Calculations have been made covering the predictions of a model representing the viscoelastic behavior of rubberlike polymers for molecular weights greater than M_c, M_c being the lower limit of the range in which the viscosity is proportional to $M^{3.4}$. A pronounced difference in the character of G'' is predicted for polymers with molecular weights between five and ten times M_c as compared with those whose molecular weights are outside this range.

In a recent publication [1] [1] we presented the steady state and transient behavior predicted by a model designed to represent the mechanical behavior, in shear, of rubberlike polymers. This model is very similar to the molecular theory of Rouse [2], except that it includes directly the effect of entanglements found in long polymer chains.

Our model assumes an entropy-type elasticity as the origin of the relaxing force observed in a stress-relaxation experiment. It involves a resistance coefficient per unit segment of a polymer chain which is evaluated from the steady state viscous behavior, and the molecular weight of the polymer, expressed as the ratio of molecular weight to critical molecular weight, M_c, defined as the lower limit of the range in which the viscosity is proportional to $M^{3.4}$.

For the particular example we presented in reference 1 this ratio was 60, and at the time we prepared this previous paper we did not have systematic calculations showing the predictions of the model for a range of molecular weights. We made an effort (sec. 3, p. 176 of reference (1)) to relate the extrema of G'' and J'' to the molecular weight through the use of various approximate relationships, since the full expressions can only be treated numerically. We have now carried out further numerical calculations covering a range of molecular weights, and find that our previous approximate relations were completely inadequate to represent the positions of these extrema as functions of molecular weight. In addition, we have found certain quite unexpected qualitative features of the predicted curves when the molecular weight is varied between one and ten times the critical molecular weight. Since these qualitative features may present the possibility of a rather critical test of the validity of this model, we present the results here in some detail.

The results of our previous paper may be represented in terms of normalized functions, the normalized modulus,

$$\mathfrak{G}^*(\gamma)=c_2G^*=\mathfrak{G}'(\theta)+i\mathfrak{G}''(\theta)$$

and the normalized compliance,

$$\mathfrak{J}^*(\gamma)=\frac{1}{c_2}J^*=\mathfrak{J}'(\theta)-i\mathfrak{J}''(\theta).$$

c_2 is a parameter equal to the kinetic theory equilibrium compliance of a vulcanized rubber with molecular weight $M_c/2$ between cross links. Obviously, these are reduced functions since the ordinary temperature and density dependence are included in c_2. γ and θ are reduced frequencies, defined by

$$\gamma=\theta(1+i)=\sqrt{i\omega c_2 r}=\sqrt{\frac{\omega c_2 r}{2}}\,(1+i)$$

where ω is the actual radian frequency and r the viscosity of a polymer of molecular weight M_c. In these terms,

$$\mathfrak{G}^*(\gamma)=\gamma\,\frac{\tanh\gamma+L\tanh K\gamma}{1+L\tanh\gamma\tanh K\gamma}=\frac{1}{\mathfrak{J}^*}, \qquad (1)$$

where

$$L=\left(\frac{l^{3.4}-1}{l-1}\right)^{1/2}, \qquad l=\frac{M}{M_c}$$

$$K=L(l-1).$$

Equation (1) represents the predictions of our model up to frequencies where the modulus is within one or two decades of the limiting high frequency modulus. This range includes all the extrema which depend on molecular weight. The maximum in G'' occurring just before G' reaches its limiting or glassy value is independent of molecular weight. Its position and magnitude can be calculated easily as given in the previous paper [1].

The calculated values of the normalized modulus and compliance as a function of the normalized frequency, θ, are shown for several values of l, used here as a measure of molecular weight, in figures

[1] Figures in brackets indicate the literature references at the end of this paper.

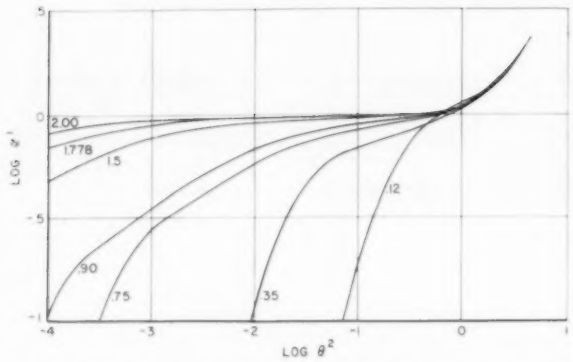

FIGURE 1. *Real part of dynamic modulus for various molecular weights.*

Parameters are values of $\log l = \log (M/M_e)$.

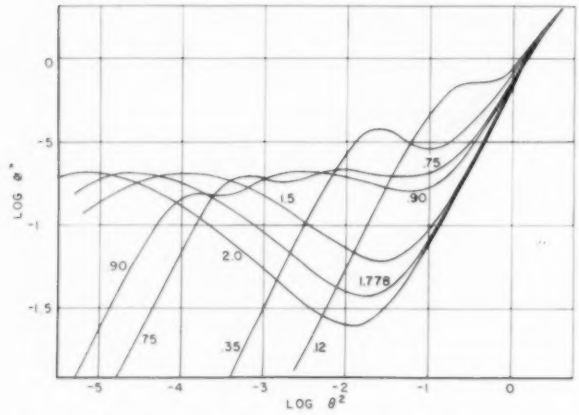

FIGURE 2. *Imaginary part of dynamic modulus for various molecular weights.*

Parameters are values of $\log l = \log (M/M_e)$.

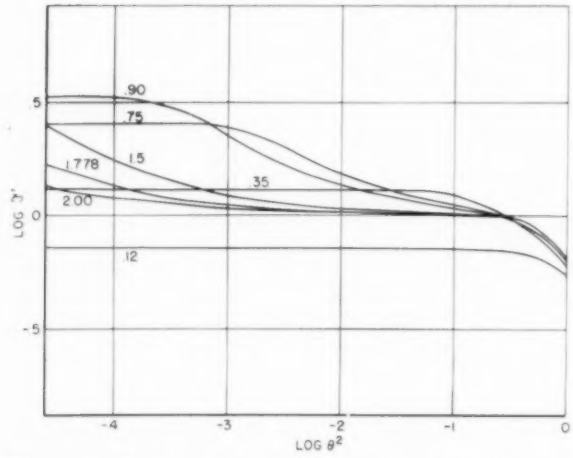

FIGURE 3. *Real part of dynamic compliance for various molecular weights.*

Parameters are values of $\log l = \log (M/M_e)$.

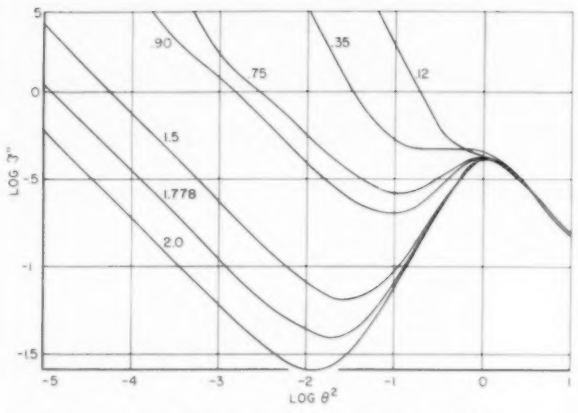

FIGURE 4. *Imaginary part of dynamic compliance for various molecular weights.*

Parameters are values of $\log l = \log (M/M_e)$.

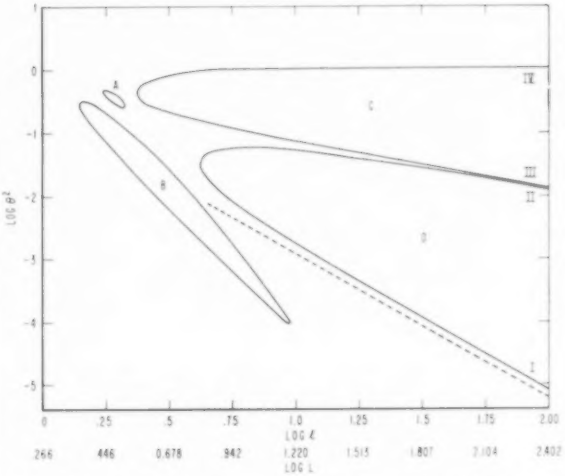

FIGURE 5. *Reduced frequencies of the extrema as a function of* $l = \frac{M}{M_e}$.

1 to 4. We see that $\mathcal{G}''$ and $\mathcal{J}''$ do not show any extrema for certain values of l, and that for other values of l there are two minima and two maxima in $\mathcal{G}''$ below the glassy range.

This occurrence of two sets of extrema was certainly unexpected. To illustrate this behavior more clearly, we show in figure 5 a plot of θ_{ext}, the frequencies at which the extrema occur, as a function of l and L. We distinguish four separate curves, A and C belonging to $\mathcal{J}''(\theta)$, B and D belonging to $\mathcal{G}''(\theta)$. The lower branches of A and C represent θ at the minimum of $\mathcal{J}''$, the upper branches θ at the maximum of that function. The lower branches of the curves B and D represent θ at the maximum of $\mathcal{G}''$ and the upper branches give θ at the minimum of that function.

The points with vertical tangents (fig. 5) correspond to inflection points of $\mathcal{G}''$ or $\mathcal{J}''$ with a horizontal tangent. This follows immediately, once we realize that they represent points where a maximum and minimum have coalesced.

It is interesting to examine the asymptotic behavior of the branches of C and D, for $l \to \infty$, since here these curves apparently become straight lines and we expect simple power laws for the functional relation between θ and l (or L). We observe from figure 5 that a common lower bound for all four branches of the curves C and D is given by

$$\theta = \frac{1}{2l^{1.2}} \sim \frac{1}{2L},$$

as indicated by the dotted line in figure 5. Hence

$$\mathrm{Re}(K\gamma) = K\theta > \frac{K}{2L} = \frac{l-1}{2} > 4.5$$

in the region $l \geq 10$, $L \geq 16.5$.

This inequality shows that $\tanh(K\gamma)$ in the expressions for $\mathcal{G}''$ and $\mathcal{J}''$ can be put equal to unity and therefore does not influence the location of any of the extrema for large l. Our functions simplify then as follows, if we introduce $\chi = \tanh^{-1}\left(\frac{1}{L}\right)$

$$\mathcal{G}''(\theta) = \mathrm{Im}\{\gamma \coth(\gamma+\chi)\} = \theta \frac{\sinh 2(\theta+\chi) - \sin 2\theta}{\cosh 2(\theta+\chi) - \cos 2\theta} \tag{2}$$

$$\mathcal{J}''(\theta) = -\mathrm{Im}\left\{\frac{1}{\gamma}\tanh(\gamma+\chi)\right\} = \frac{1}{2\theta}\frac{\sinh 2(\theta+\chi) - \sin 2\theta}{\cosh 2(\theta+\chi) + \cos 2\theta} \tag{3}$$

We turn now to the determination of the asymptotic behavior of the branches I, II, III, IV. On both branches I and II of curve D, θ and χ approach zero as L increases. We can thus use Taylor's expansion to obtain:

$$\mathcal{G}'' = \frac{\theta\chi}{2\theta^2 + 2\chi\theta + \chi^2} + \frac{1}{3}\theta(2\theta+\chi) + O(\theta^3).$$

The derivative of the first term (with respect to θ) predicts a maximum at $\theta_{max} = \frac{\chi}{\sqrt{2}} = \frac{1}{2^{1/2}L}\left(\chi \approx \frac{1}{L} \text{ for large } L\right)$ with $\mathcal{G}''_{max} = 0.207$. This is the only extremum predicted by the first term alone. To find a condition for the minimum we re-write the above as:

$$\mathcal{G}'' = \frac{\chi}{2\theta}\left(1 - \frac{\chi}{\theta} + \frac{\chi^2}{2\theta^2} + \dots\right) + \frac{2}{3}\theta^2\left(1 + \frac{\chi}{2\theta}\right) + O(\theta^3),$$

this expression being permitted because on branch II $\chi \ll \theta^2$. This latter relation justifies our taking, for large L,

$$\mathcal{G}'' \approx \frac{\chi}{2\theta} + \frac{2}{3}\theta^2.$$

From which we predict a minimum at

$$\theta_{min} = \left(\frac{3}{8L}\right)^{1/3}$$

with a magnitude

$$\mathcal{G}''_{min} = 1.04L^{-2/3}.$$

An expression for the asymptote of the minimum in $\mathcal{J}''$ represented by branch III (curve C) may be obtained from a similar expansion of $\tanh(\gamma+\chi)$, again retaining two terms and using the fact that $\chi < \theta^2$. It yields, as is apparent from figure 5, the same value as the asymptote for branch II:

$$\mathcal{J}'' \approx \frac{\chi}{2\theta} + \frac{2}{3}\cdot\theta^2,$$

from which

$$\theta_{min} = \left(\frac{3}{8L}\right)^{1/3},$$

and

$$\mathcal{J}''_{min} = 1.04L^{-2/3}.$$

The maximum in $\mathcal{J}''$, branch IV of curve C, appears to be nearly independent of l. If it were strictly independent, it would be the maximum of:

$$\frac{1}{2\theta}\cdot\frac{\sinh 2\theta - \sin 2\theta}{\cosh 2\theta + \cos 2\theta},$$

the asymptotic expression corresponding to eq (3) for large l. This function has a maximum value of

$$\mathcal{J}''_{max} = 0.4172$$

at

$$\theta_{max} = 1.127.$$

The following tabulation shows that these maxima of our calculated $\mathcal{J}''$ functions depend only very slightly on l:

for $l = 5.012$: $\mathcal{J}''_{max} = 0.4325$, $\theta_{max} = 1.019$

for $l = 100.00$: $\mathcal{J}''_{max} = 0.4178$, $\theta_{max} = 1.122$.

It is difficult to do more than point out the existence of curves A and B (fig. 5), which was not even suspected prior to these detailed numerical calculations. Since in this region $\tanh K\gamma$ cannot be taken as unity, the analytic expressions for $\mathcal{G}''$ and $\mathcal{J}''$ are very complicated. There is no reason to expect that expressions for curves A and B would be simple enough to be useful. Therefore we leave them with the presentation of the numerical results. These computations have now been carried out in sufficient detail that we are essentially certain we have found all the extrema predicted by the model for both $\mathcal{G}''$ and $\mathcal{J}''$.

The behavior of $\mathfrak{G}'$ and $\mathfrak{G}''$ calculated here as a function of molecular weight should provide a critical test of our model if appropriate experimental data could be found for comparison. In the molecular weight range of about 5 to 10 times M_e this model predicts an essentially constant value of G'' over two to three decades of frequency, with G' increasing fairly steadily over the same range. For higher molecular weights the G'' curve should show a pronounced maximum and minimum, their separation becoming greater on both the frequency and modulus scales with increasing molecular weight. In the vicinity of the minimum of G'', G' should remain fairly constant. Since we do not know how a distribution of molecular weights should be introduced into our model, it would be preferable to make the comparison with experimental measurements on fractionated materials, but lacking such data it seems most reasonable to use a weight average molecular weight.

While we do not know of any dynamic measurements which can be used to check these predictions directly, the stress relaxation measurements and calculated relaxation spectra reported by Tobolsky and Murakami [3] for a series of polystyrene samples with weight average molecular weights ranging from $4.25\times10^4(=1.1\ M_e)$ to $3.15\times10^5(=8.3\ M_e)$ (their sample numbers 6 to 15) and $\overline{M}_w/\overline{M}_n=1.5$ represent a reasonable check on the predictions summarized above. The stress relaxation modulus is approximately the mirror image of G', and the spectrum $\overline{H}(\tau)$ is, to a zero order approximation, equal to $(2/\pi)G''(1/\tau)$.

The graphs of $\overline{H}$ shown in figure 4 of reference 3 show no plateau region for molecular weights between M_e and 2.4 M_e (samples 6 to 11). Distinct plateau regions are seen for samples with molecular weights between 3.2 M_e and 8.3 M_e (samples 12 to 15). For all these samples the $G(t)$ curves are monotonically decreasing, with no hint of a plateau region. For higher molecular weights, of course, we normally find a region where $G(t)$ or $G'(\omega)$ are changing so slowly as to suggest strongly a plateau. This type of behavior is observed in our calculated curves for $l>15$.

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(Paper 67B2–96)

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Selected Bibliography of Statistical Literature: Supplement, 1958–1960

Lola S. Deming

(February 8, 1963)

This is the last of a series of bibliographies that deal with various specific subjects in the field of statistics. The preceding six bibliographies of the series gave references for the period from 1930 to 1957. This one is intended to supplement the others by bringing them up to date through 1960. The references are arranged under the various subject titles published earlier in this series.

The purpose of this series of bibliographies is to provide a list of references in several specific subjects within the very large field of probability and mathematical statistics. The purpose of this last one in the series is to supplement the others by including references to related material published in 1958, 1959, and 1960. We felt that to carry this effort beyond 1960 would be redundant and overlapping. Within the last few years a number of bibliographic resources have become available in varying degrees of generality and specialization either as one-volume lists of references or as continuing abstract services. Although my intention is not to give a bibliography of bibliographies and abstract services, I shall mention several significant ones to show that as the statistical literature grows to a staggering amount, so also does interest grow in the construction of reference material to make the statistician aware of the existence of papers relevant to his field and to enable him to trace them.

Most noteworthy among the bibliographies is the *Bibliography of Statistical Literature 1950–1958* by Maurice G. Kendall and Alison G. Doig. Professor Kendall promises that two more volumes, also covering the general field of statistical method and theory, will follow to cover the period from the 16th century up to 1950. A number of excellent bibliographies that specialize in particular phases of statistics have also been published. Two of these cover subjects that were intended for inclusion within this present series. However, in each case the author did a more thorough search of the literature for his particular area than could have been handled here. These are: I. Richard Savage, *Bibliography of Nonparametric Statistics*, Harvard University Press, Cambridge, Mass., 1962; and J. Edward Jackson, *Bibliography on Sequential Analysis*, Jour. Amer. Stat. Assoc. Vol. 55, 561–580, Sept. 1960.

A great service to the statistician is provided by the International Statistical Institute through its two abstracting journals: *International Journal of Abstracts—Statistical Theory and Methods*, published quarterly since 1959; and *International Journal of Abstracts—Statistical Methods in Industry* published three times a year since 1954. Another digest service in applied statistics is *Quality Control and Applied Statistics* published by Interscience Publishers, Inc., New York.

As was explained in other sections of this series, we have limited the source material to the two large reviewing journals—*Zentralblatt für Mathematik* for the years 1930–1939, and *Mathematical Reviews* from 1940–1960. All abstracts under the general headings of "Probability" and "Mathematical Statistics" are transferred to cards. These are arranged alphabetically by author and placed in a file. This collection of abstracts is maintained on a current basis in the NBS Statistical Engineering Laboratory. The abstracts are coded into many categories of subject matter following generally, but with some minor deviations, the classification scheme of *Mathematical Reviews*. One abstract may be classified under several subjects; hence it may appear in more than one place in this series. References were transcribed from the abstracts by means of punched cards and titles were added to prepare the following selected subjects for publication in the *NBS Journal of Research:*

Correlation and Regression Theory, Vol. 64B, pp. 55–68, January–March 1960;
Time Series, Vol. 64B, pp. 69–76, January–March 1960;
Limit Theorems, Vol. 64B, pp. 175–192, July–September 1960;
Markov Chains and Stochastic Processes, Vol. 65B, pp. 61–93, January–March 1961;
Frequency Functions, Moments, and Graduation, Vol. 66B, pp. 15–28, January–March 1962;
Theory of Estimation and Testing of Hypotheses, Sampling Distributions, and Theory of Sample Surveys, Vol. 66B, pp. 109–151, July–September 1962.

Most of the abstracts deal with statistical theory and methodology with applications usually appearing only when they illustrate something new or novel in theory or method. The classification scheme for the *Mathematical Reviews* has undergone revision from time to time and in the last several years the category "Correlation and Regression Theory" was eliminated entirely and articles on these subjects placed among the other classifications as appropriate.

The references given here contain the following information taken directly from the abstracts:

Author: The author's surname, followed by initials only. In the case of multiple authorships, the journal reference appears with each author's name, but the title of the paper appears with the first author only. The symbol ♦ preceding the surname denotes multiple authorship.

Title: Exactly as in the reviewing journal. Titles of separately bound publications (books, reports, theses, etc.) are in italics, followed by the publisher.

Reference to literature: The name of the journal in italics and the number of the volume in bold face, are followed by initial page number.

Date of publication: The next figure, in parentheses shows the date when the article or book itself appeared.

M (for *Mathematical Reviews*) and Z (for *Zentralblatt für Mathematik*) are followed by the volume number and page number of the reviewing journal in which the abstract appears.

Time Series

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(Paper 67B2–97)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 67B, No. 2, April–June 1963

Publications of The National Bureau of Standards*

Selected Abstracts

Perturbation method in a problem of waveguide theory, D. Fox and W. Magnus, *J. Research NBS* **67D** (Radio Prop.) *No. 2, 189 (Mar.–Apr. 1963). 70 cents.*
The reflection coefficient for the basic mode in a widening, straight, two-dimensional waveguide is computed for small wave numbers by using the perturbation method with the electrostatic case as the unperturbed case. The problem is treated as a perturbed infinite system of inhomogeneous linear equations, and it is shown that the matrix of the unperturbed system (which corresponds to the electrostatic case) can be inverted explicitly by using conformal mappings and physically unrealistic modes. Questions of convergence are discussed, and other examples for application of the method are indicated.

Some wave functions and potential functions pertaining to spherically stratified media, C. T. Tai, *J. Research NBS* **67D** (Radio Prop.) *No. 2, 199 (Mar.–Apr. 1963). 70 cents.*
The wave functions pertaining to a bilinearly stratified medium are presented in this paper. Solutions to the equation $\nabla\cdot[\kappa(r)\nabla\Psi]=0$ have been investigated for several profiles of $\kappa(r)$. An analysis is given to the equation $\nabla\cdot[\kappa\cdot\nabla\Psi]=-\rho/\epsilon_0$ which arises from the formulation of the quasi-static electric field in a homogeneous anisotropic medium.

Relative convergence of the solution of a doubly infinite set of equations, R. Mittra, *J. Research NBS* **67D** (Radio Prop.) *No. 2, 245 (Mar.–Apr. 1963). 70 cents.*
The paper deals with the relative convergence of a doubly-infinite set of equations pertaining to a boundary value problem in a waveguide. It is shown that the solution for the equations converges differently for different choices of the combination of the number of equations from the two sets. This is demonstrated by studying the convergence properties of the truncated set of equations as the number of equations is made indefinitely large. It is proven that the solution for the reflection coefficient becomes identical with the exact solution only with a particular choice of the ratio of the equations. This choice of the unique ratio is also shown to be consistent with the edge condition.

Realistic diatomic potential function, H. W. Woolley, *J. chem. Phys.* **37,** *No. 6, 1307–1316 (Sept. 1962).*
An examination of recently published data for diatomic molecules as obtained by the Rydberg-Klein-Rees method has suggested a useful form for the potential-energy function. This form provides an inverse-power dependence at large distance and an extrapolation to infinity at the extreme of close approach. Relations are given to permit an arbitrarily close fit of observed spectroscopic constants. Theoretical formulas covering seven new $Y[_{ll}]$'s of the Dunham–Sandeman series for the rotating vibrator are included. Potential curves for H_2 and HF are shown as examples, including effects of previously determined higher-order spectroscopic constants. Other applications of the new potential are also discussed.

Tests for contingency tables and Markov chains, S. Kullback, M. Kupperman, and H. H. Ku, *Technometrics* **4,** *No. 4, 573–608 (Nov. 1962).*
A number of useful tests for contingency tables and finite stationary Markov chains are presented in this paper based on the use of the notions of information theory. A consistent and simple approach is used in developing the various test procedures and the results are given in the form of analysis-of-information tables. Beginning with tests of hypotheses for a one-way table, tests of hypotheses of specified probabilities, independence, conditional independence, homogeneity of classifications, and symmetry are developed for contingency tables of two, three, four, and higher order classifications. For the Markov chains, the tests include the hypotheses of a specified matrix of transition probabilities, Markovity, and homogeneity of several realizations of Markov chains. Worked examples are given throughout the paper. A table of $2n \ln n$ for $n=1$ (1) 10,000 is appended for use in computation.

A molecular-orbital study of the geometry of HO_2, M. E. Boyd, *J. Chem. Phys.* **37,** *No. 6, 1317–1325 (Sept. 1962).*
Determination of the energy of HO_2 as a function of the HO_1O_2 angle for fixed values of $R(H—O_1)$ and $R(H—O_2)$ has been carried out using LCAO–MO–SCF calculations on closed-shell ions. All one-electron and one- and two-center two-electron integrals used were evaluated accurately while three-center integrals were approximated. An isosceles-triangle configuration is favored by these calculations and gives a value of the ionization potential of 9.5 eV and dissociation energy of 4.4 eV, consonant with experimental results. Approximation by means of ionic calculations used here is shown to be valid for the purposes of this discussion.

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Pressure-density-temperature relations of fluid para hydrogen from 15 to 100 °K at pressures to 350 atmospheres. R. D. Goodwin, D. E. Diller, H. M. Roder, and L. A. Weber.
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